CHAPTER III

Roots of Equations

The objective of this chapter is to introduce methods to solve linear and non-linear equations. We will see how do these methods work and compute their errors.

I. GRAPHICAL METHODS

This is the simplest method to determine the root of an equation $f(x) = 0$.
The procedure is quite straightforward:

- Plot the function $f(x)$
- Observe when it crosses the x-axis, this point represents the value for which $f(x) = 0$.

Note 1: This will provide only a rough approximation of the root.
Note 2: you can remark that the function has changed sign after the root.

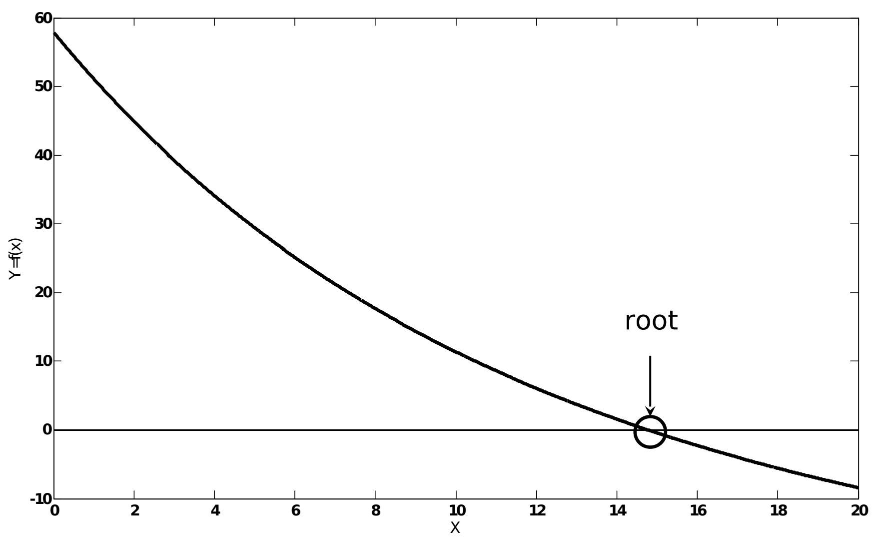


Figure.3.1. graphical method.

However, this rough approximation of the root can be used as a first guess for other more accurate techniques.

BRACKETING METHODS

II. Bisection method

One of the first numerical methods developed to find the root of a nonlinear equation $f(x)=0$ was the bisection method (also called Binary-Search method). The method is based on the following theorem:

> **Theorem:** An equation $f(x)=0$, where $f(x)$ is a real continuous function, has at least one root between x_ℓ and x_u if $f(x_\ell)\,f(x_u)<0$ (Figure 3.2).
> Note that if $f(x_\ell)\,f(x_u)>0$, there may or may not be any root between x_ℓ and x_u (Figures 3.3 and 3.4). If $f(x_\ell)\,f(x_u)<0$, then there may be more than one root between x_ℓ and x_u (Figure 3.5). So the theorem only guarantees one root between x_ℓ and x_u.

Since the method is based on finding the root between two points, the method falls under the category of bracketing methods.

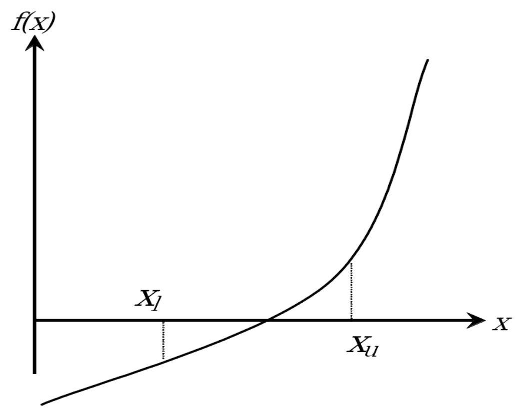


Figure.3.2. At least one root exists between two points if the function is real, continuous, and changes sign.

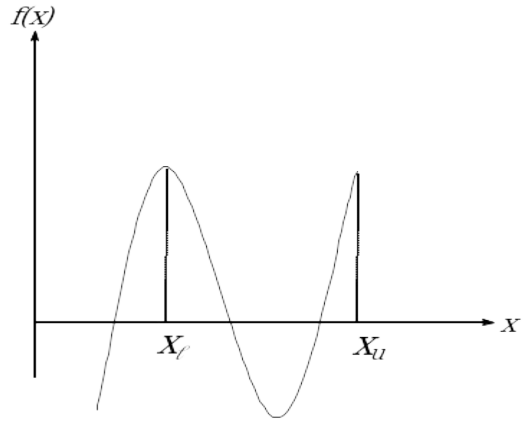


Figure.3.3. If function $f(x)$ does not change sign between two points, roots of $f(x)=0$ may still exist between the two points.

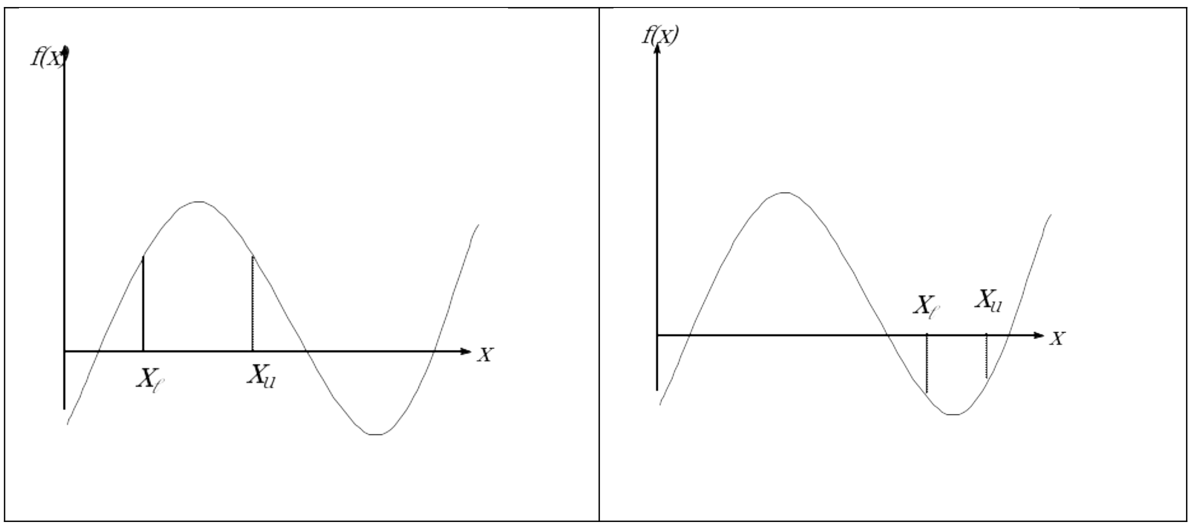


Figure.3.4. If the function $f(x)$ does not change sign between two points, there may not be any roots $f(x)=0$ between the two points.

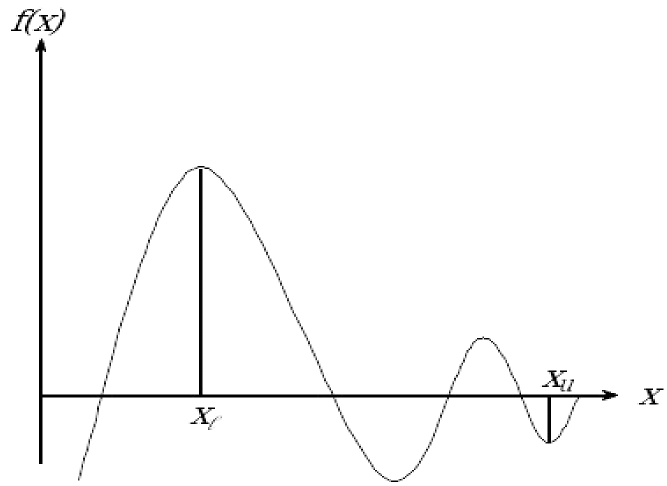


Figure.3.5. If the function $f(x)$ changes sign between two points, more than one root for $f(x) = 0$ may exist between the two points.

A general rule is:

- If the f(x_l) and f(x_u) have the same sign ($f(x_\ell)\,f(x_u) > 0$):
    - There is no root between x_l and x_u.
    - There is an even number of roots between x_l and x_u.

- If the f(x_l) and f(x_u) have different signs ($f(x_\ell)\,f(x_u) < 0$):
    - The is an odd number of roots.

Exceptions:

- Multiple roots

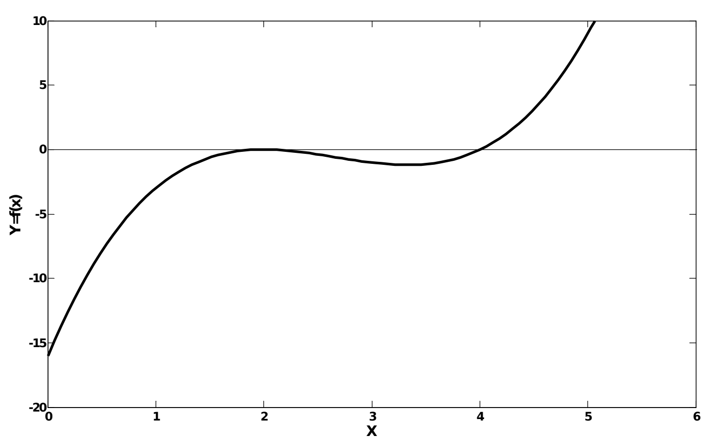


Figure.3.6. Multiple roots.

Example: $f(x) = x^3 + x^2 - 5x + 3 \Leftrightarrow f(x) = (x+3)(x-1)^2$

- Discontinuous functions

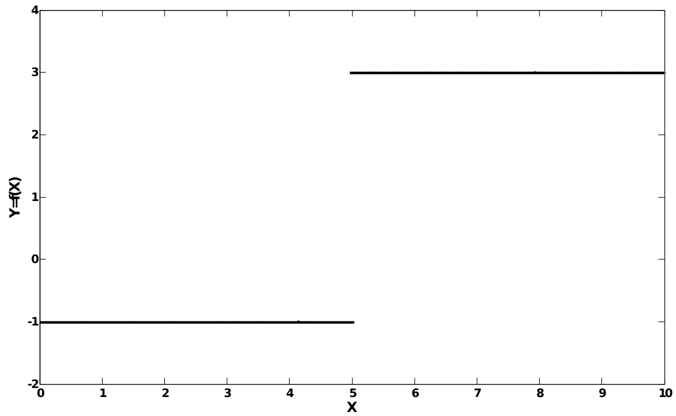


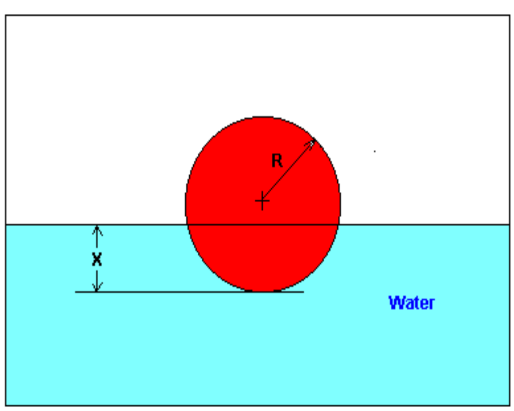
Figure.3.7. Discontinuous function.

The steps to apply the bisection method to find the root of the equation $f(x) = 0$ are:

1. Choose x_ℓ and x_u as two guesses for the root such that $f(x_\ell)\,f(x_u) < 0$, or in other words, $f(x)$ changes sign between x_ℓ and x_u.
2. Estimate the root, x_m of the equation $f(x) = 0$ as the mid-point between x_ℓ and x_u as
$$x_m = \frac{x_\ell + x_u}{2}$$
3. Now check the following
   a. If $f(x_\ell)\,f(x_m) < 0$, then the root lies between x_ℓ and x_m; then $x_\ell = x_\ell$ and $x_u = x_m$.
   b. If $f(x_\ell)\,f(x_m) > 0$, then the root lies between $x_m$and x_u; then $x_\ell = x_m$and $x_u = x_u$.
   c. If $f(x_\ell)\,f(x_m) = 0$; then the root is x_m. Stop the algorithm if this is true.
4. Find the new estimate of the root
$$x_m = \frac{x_\ell + x_u}{2}$$
Find the absolute approximate relative error as
$$|\varepsilon_a| = \left|\frac{x_m^{new} - x_m^{old}}{x_m^{new}}\right| \times 10($$
where
x_m^{new} = estimated root from present iteration
x_m^{old} = estimated root from previous iteration
5. Compare the absolute relative approximate error $|\varepsilon_a|$ with the pre-specified relative error tolerance ε_s. If $|\varepsilon_a| > \varepsilon_s$, then go to Step 3, else stop the algorithm. Note one should also check whether the number of iterations is more than the maximum number of iterations allowed. If so, one needs to terminate the algorithm and notify the user about it.

Example

A ball has a specific gravity of 0.6 and has a radius of 5.5 cm. What is the distance to which the ball will get submerged when floating in water?



The equation that gives the depth 'x' to which the ball is submerged under water is:

$$x^3 - 0.165x^2 + 3.993\times10^{-4} = 0$$

II.2. Advantages and drawbacks of the bisection method

II.2.1. Advantages of Bisection Method

a) The bisection method is always convergent. Since the method brackets the root, the method is guaranteed to converge.

b) As iterations are conducted, the interval gets halved. So one can guarantee the decrease in the error in the solution of the equation.

II.2.2. Drawbacks of Bisection Method

a) The convergence of bisection method is slow as it is simply based on halving the interval.

b) If one of the initial guesses is closer to the root, it will take larger number of iterations to reach the root.

c) If a function $f(x)$ is such that it just touches the x-axis (Figure 3.8) such as

$$f(x) = x^2 = 0$$

it will be unable to find the lower guess, x_ℓ, and upper guess, x_u, such that

$$f(x_\ell)\, f(x_u) < 0$$

d) For functions $f(x)$ where there is a singularity[1] and it reverses sign at the singularity, bisection method may converge on the singularity (Figure 3.9). An example include

$$f(x) = \frac{1}{x}$$

and $x_l = -2$, $x_u = 3$ are valid initial guesses which satisfy

$$f(x_\ell)\, f(x_u) < 0.$$

However, the function is not continuous and the theorem that a root exists is also not applicable.

[1] A singularity in a function is defined as a point where the function becomes infinite. For example, for a function such as 1/x, the point of singularity is x=0 as it becomes infinite.

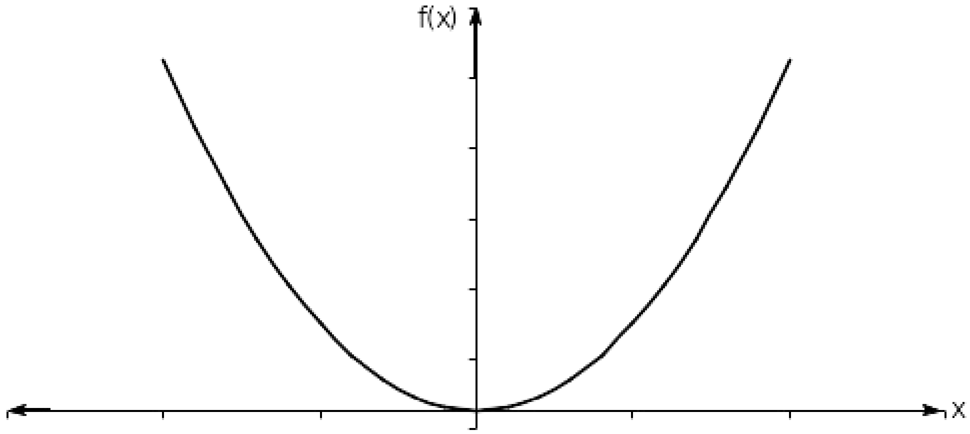


Figure.3.8. Function $f(x) = x^2 = 0$ has a single root at $x = 0$ that cannot be bracketed.

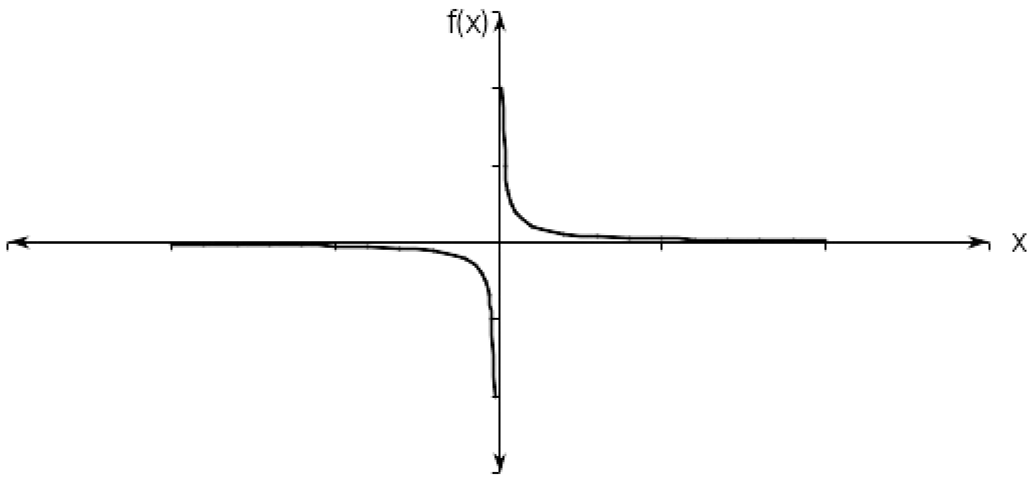


Figure.3.9. Function $f(x) = \frac{1}{x} = 0$ has no root but changes sign.

III. False position method

A shortcoming of the bisection method is that in dividing the interval from x_l to x_u into equal halves, no account is taken of the magnitude of $f(x_i)$ and $f(x_u)$. Indeed, if $f(x_i)$ is close to zero, the root is more close to x_l than x_0.

The false position method uses this property:
A straight line joins $f(x_i)$ and $f(x_u)$. The intersection of this line with the x-axis represents an improvement estimate of the root. This new root can be computed as:

$$\frac{f(x_l)}{x_r - x_l} = \frac{f(x_u)}{x_r - x_u}$$

Giving $$x_r = x_u - \frac{f(x_u)(x_l - x_u)}{f(x_l) - f(x_u)}$$ This is called the false-position formula

Then, x_r replaces the initial guess for which the function value has the same sign as $f(x_r)$

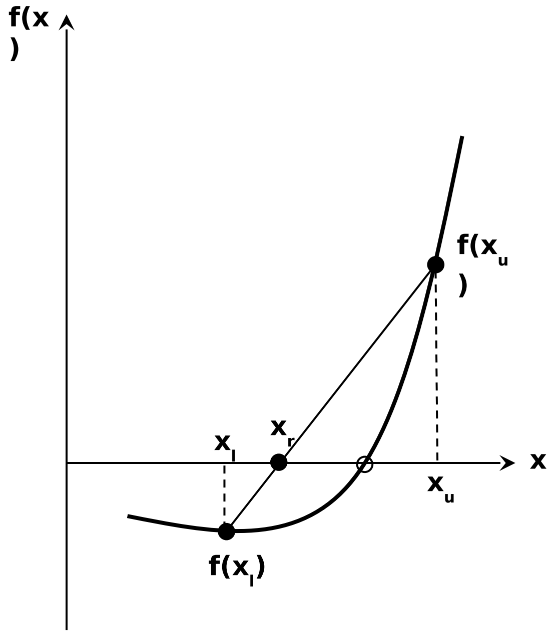


Figure.3.10. False-position method.

The difference between bisection method and false-position method is that in bisection method, both limits of the interval have to change. This is not the case for false position method, where one limit may stay fixed throughout the computation while the other guess converges on the root.

III.1. Pitfalls of the false-position method

Although, the false position method is an improvement of the bisection method. In some cases, the bisection method will converge faster and yields to better results (see Figure.3.11).

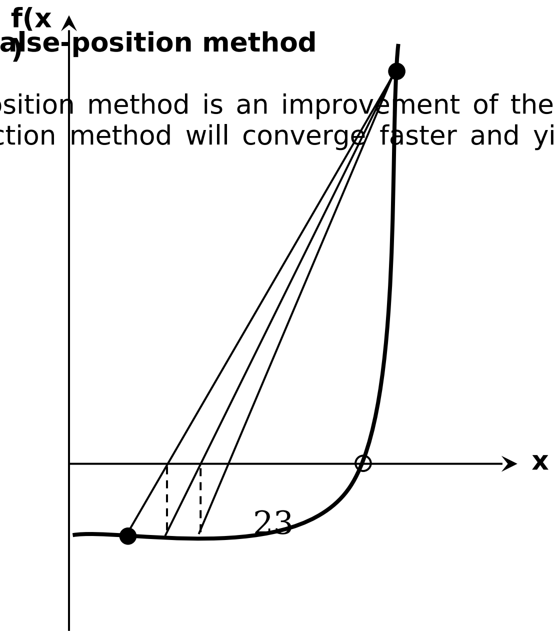


Figure.3.11. Slow convergence of the false-position method.

IV. Modified false position method

As the problem with the original false-position method is the fact that one limit may stay fixed during the computation, we can introduce a modified method in which if one limit is detected to be stuck, the function value of the stagnant point is divided by 2.

V. Incremental searches and determining initial guesses

To determine the number of roots within an interval, it is possible to use an incremental search. The function is scanned from one side to the other using a small increment. When the function changes sign, it is assumed that a root falls within the increment.

The problem is the choice of the increment length:

Too small	very time consuming
Too large	some root may be missed

The solution is to use plotting or information from the physical problem.

OPEN METHODS

Bracketing methods use two initial guesses and the bounds converge to the solution. In open methods, we need only one starting point or two (that not necessarily bracket the root).
These methods may diverge, contrary to the bracketing methods, but when they converge, they usually do it much more quickly than bracketing methods.

VI. Simple fixed-point method

In open methods, we have to use a formula to predict the root, as an example for the fixed-point iteration method we can rearrange f(x) so that x is on the left-hand side of the equation:

$$x = g(x)$$

This can be achieved by algebraic manipulation of by simply adding x to both sides of the original equation, example:

$$x^2 + 3x - 1 = 0 \Leftrightarrow x = \frac{1 - x^2}{3}$$
$$\sin(x) = 0 \Leftrightarrow x = \sin(x) + x$$

This is important since it will allow us to develop a formula to predict the new value for x as a function of an old value of x:

$$x_{i+1} = g(x_i)$$

VI.1. Convergence

VII. Newton-Raphson method

Newton-Raphson method is based on the principle that if the initial guess of the root of f(x)=0 is at x_i, then if one draws the tangent to the curve at $f(x_i)$, the point x_{i+1} where the tangent crosses the x-axis is an improved estimate of the root (Figure 3.12).
Using the definition of the slope of a function, at $x = x_i$

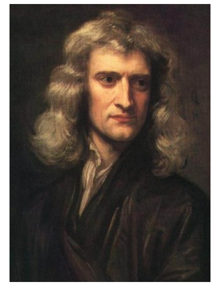
$$f(x_i) = = \frac{f(x_i) - 0}{x_i - x_{i+1}}$$

which gives

$$x_{i+1} = x_i - \frac{f(x_i)}{f'(x_i)}$$

This equation is called the Newton-Raphson formula for solving nonlinear equations of the form $f(x) = 0$. So starting with an initial guess, x_i, one can find the next guess, x_{i+1}, by using the above equation. One can repeat this process until one finds the root within a desirable tolerance.

Sir Isaac Newton, (4 January 1643 – 31 March 1727) [OS: 25 December 1642 – 20 March 1727] was an English physicist, mathematician, astronomer, alchemist, and natural philosopher, regarded by many as the greatest figure in the history of science.[2] His treatise *Philosophiae Naturalis Principia Mathematica*, published in 1687, described universal gravitation and the three laws of motion, laying the groundwork for classical mechanics. By deriving Kepler's laws of planetary motion from this system, he was the first to show that the motion of objects on Earth and of celestial bodies are governed by the same set of natural laws. The unifying and predictive power of his laws was integral to the scientific revolution, the advancement of heliocentrism, and the broader acceptance of the



Joseph Raphson was an English mathematician known best for the Newton-Raphson method. Little is known about Raphson's life- even his exact birth and death years are unknown, though the mathematical historian Florian Cajori supplied the approximate dates 1648-1715. Raphson attended Jesus College in Cambridge and graduated with an M.A. in 1692. Raphson was made a Fellow of the Royal Society in 30 November 1689 after being proposed for membership by Edmund Halley.

Raphson's most notable work was *Analysis Aequationum Universalis* which was published in 1690. It contained the Newton-Raphson method for approximating the roots of an equation. Isaac Newton developed the same formula in the *Method of Fluxions*. Although Newton's work was written in 1671, it was not published until 1736- nearly 50 years after Raphson's *Analysis*.

Algorithm

The steps to apply using Newton-Raphson method to find the root of an equation f(x) = 0 are

1. Evaluate $f'(x)$ symbolically
2. Use an initial guess of the root, x_i, to estimate the new value of the root x_{i+1} as

$$x_{i+1} = x_i - \frac{f(x_i)}{f'(x_i)}$$

3. Find the absolute relative approximate error, $|\varepsilon_a|$ as

$$|\varepsilon_a| = \left|\frac{x_{i+1} - x_i}{x_{i+1}}\right| \times 100$$

4. Compare the absolute relative approximate error, $|\varepsilon_a|$ with the pre-specified relative error tolerance, ε_s. If $|\varepsilon_a| > \varepsilon_s$, then go to step 2, else stop the algorithm. Also, check if the number of iterations has exceeded the maximum number of iterations.

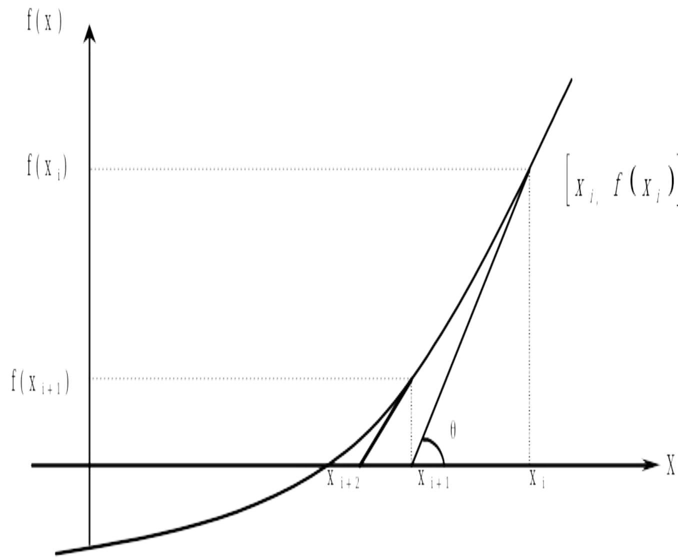


Figure.3.12. Geometrical illustration of the Newton-Raphson method.

Example

Solve the same problem for the floating ball using Newton-Raphson method. Find:

a) the depth 'x' to which the ball is submerged under water. Conduct three iterations to estimate the root of the above equation.

find the absolute relative approximate error at the end of each iteration.

VI.1. Drawbacks of Newton-Raphson Method

- Divergence at inflection points: If the selection of a guess or an iterated value turns out to be close to the inflection point of f(x), that is, near where f"(x)=0, the roots start to diverge away from the true root.

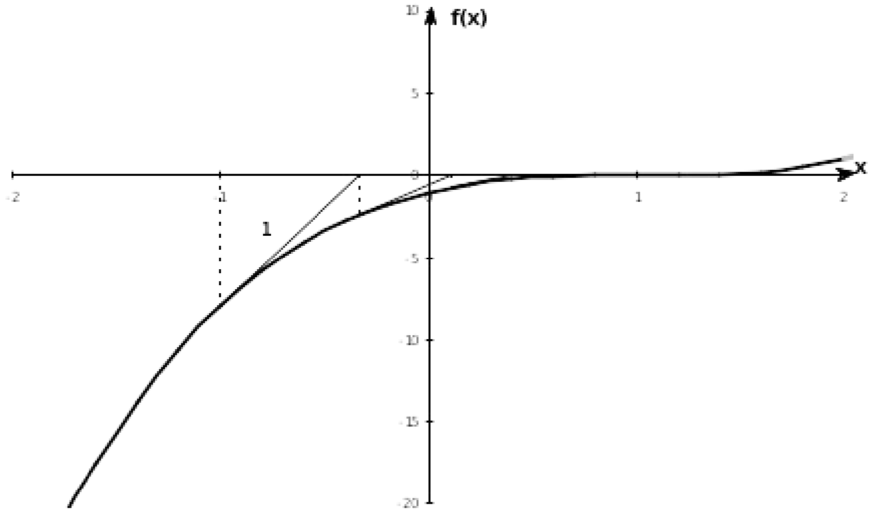


Figure.3.13. Divergence at inflection point.

- Division by zero or near zero: The formula of Newton-Raphson method is

$$x_{i+1} = x_i - \frac{f(x_i)}{f'(x_i)}$$

Consequently if an iteration value, x_i is such that $f'(x_i) \cong 0$, then one can face division by zero or a near-zero number. This will give a large magnitude for the next value, x_{i+1}. An example is finding the root of the equation

$$f(x) = x^3 - 0.03x^2 + 2.4\times10^{-6}$$

in which case

$$f'(x) = 3x^2 - 0.06x$$

For $x_0 = 0$ or $x_0 = 0.02$, division by zero occurs (Figure 3.14). For an initial guess close to 0.02, of $x_0 = 0.0199$, even after 9 iterations, the Newton-Raphson method is not converging.

Iteration Number	x_i	$\lvert\varepsilon_a\rvert$	$f(x_i)$
0	0.019990		-1.6000×10^{-6}
1	-2.6480	100.75	-18.778
2	-1.7620	50.282	-5.5638
3	-1.1714	50.422	-1.6485
4	-0.77765	50.632	-0.48842
5	-0.51518	50.946	-0.14470
6	-0.34025	51.413	-0.042862
7	-0.22369	52.107	-0.012692
8	-0.14608	53.127	-0.0037553
9	-0.094490	54.602	-0.0011091

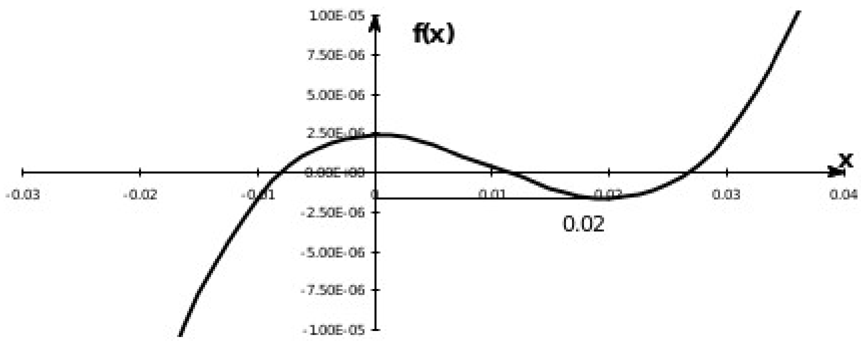


Figure 3.14. Division by zero or a near zero number.

- Root jumping: In some case where the function f(x) is oscillating and has a number of roots, one may choose an initial guess close to a root. However, the guesses may jump and converge to some other root. For example for solving the equation

$$\sin x = 0$$

if you choose $x_0 = 2.4\pi = (7.539822)$ as an initial guess, it converges to the root of x=0 as shown in Table 3. However, one may have chosen this an initial guess to converge to $x = 2\pi = 6.2831853$.

Iteration Number	x_i	**f(x$_i$)**	$\lvert\epsilon_a\rvert$
0	7.539822	0.951	
1	4.461	-0.969	68.973
2	0.5499	0.5226	711.44
3	-0.06303	-0.06303	971.91
4	6.376×10^{-4}	8.375×10^{-4}	7.54×10^{4}
5	-1.95861×10^{-13}	-1.95861×10^{-13}	4.27×10^{10}

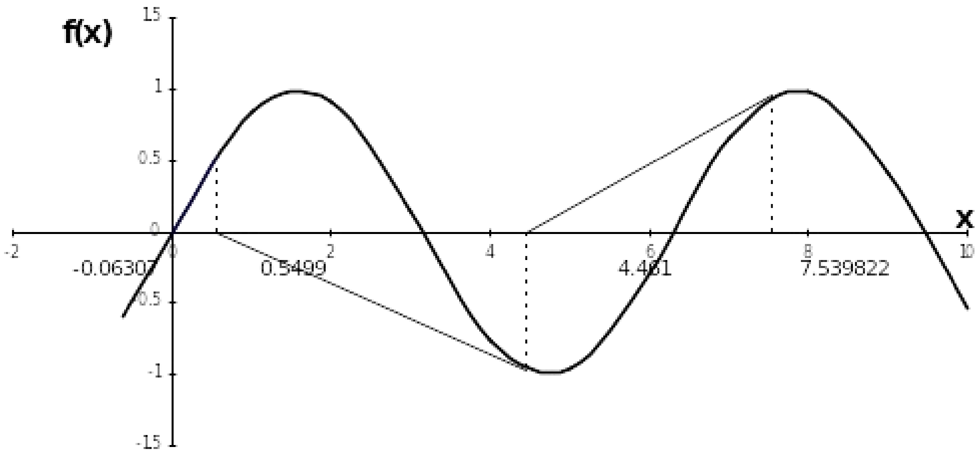


Figure 3.15. Root jumping from intended location of root for $f(x) = \sin x = 0$

- Oscillations near local maximum and minimum: Results obtained from Newton-Raphson method may oscillate about the local maximum or minimum without converging on a root but converging on the local maximum or minimum. Eventually, it may lead to division by a number close to zero and may diverge. For example for

$$f(x) = x^2 + 2 = 0$$

the equation has no real roots

Iteration Number	x_i	**f(x$_i$)**	$\lvert\varepsilon_a\rvert$
0	-1.0000	3.00	
1	0.5	2.25	300.00
2	-1.75	5.062	128.571
3	-	2.092	476.47
4	0.30357	11.874	109.66
5	3.1423	3.57	150.80
6	1.2529	2.029	829.88

7	-	34.942	102.99
8	0.17166	9.268	112.927
9	5.7395	2.954	175.96
	2.6955		
	0.9770		

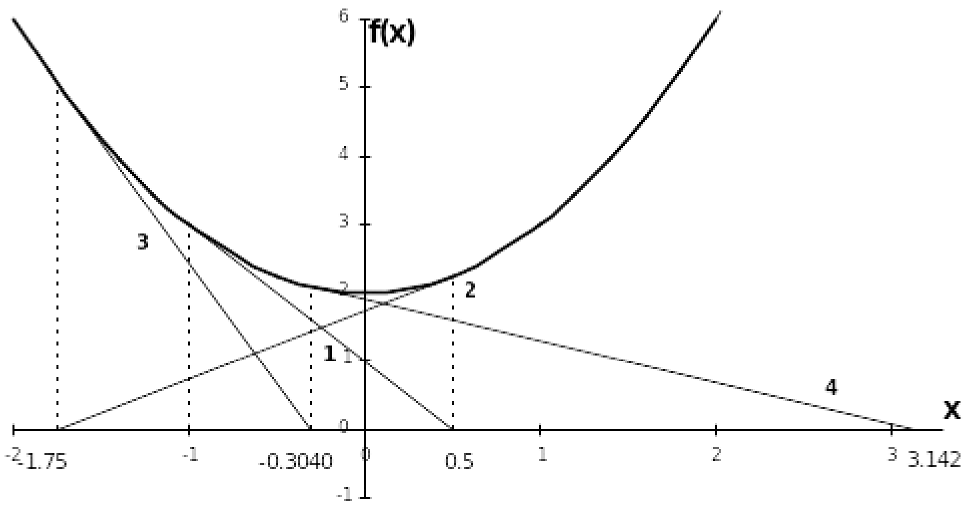


Figure.3.16. Oscillations around local minima for $f(x) = x^2 + 2$

VI.2. Additional features for Newton-Raphson

- Plot your function to correctly choose the initial guess.
- **Substitute your solution into the original function.**
- **Substitute your solution into the original function.**
- **Substitute your solution into the original function.**
- **Substitute your solution into the original function.**
- **Substitute your solution into the original function.**
- **Substitute your solution into the original function.**
- **Substitute your solution into the original function.**
- The program must always include an upper limit on the number of iterations.
- The program should alert the user of the possibility of $f'(x) = 0$.

VII. The secant method

The Newton-Raphson method of solving the nonlinear equation f(x)=0 is given by the recursive formula

$$x_{i+1} = x_i - \frac{f(x_i)}{f'(x_i)} \tag{1}$$

From the above equation, one of the drawbacks of the Newton-Raphson method is that you have to evaluate the derivative of the function. With availability of symbolic manipulators such as Maple, Mathcad, Mathematica and Matlab, this process has become more convenient. However, it is still can be a laborious process. To overcome this drawback, the derivative, f'(x) of the function, f(x) is approximated as

$$f'(x_i) = \frac{f(x_i) - f(x_{i-1})}{x_i - x_{i-1}} \tag{2}$$

Substituting Equation (2) in (1), gives

$$x_{i+1} = x_i - \frac{f(x_i)(x_i - x_{i-1})}{f(x_i) - f(x_{i-1})}$$

(3)

The above equation is called the Secant method. This method now requires two initial guesses, but unlike the bisection method, the two initial guesses do not need to bracket the root of the equation. The Secant method may or may not converge, but when it converges, it converges faster than the bisection method. However, since the derivative is approximated, it converges slower then Newton-Raphson method.

The Secant method can be also derived from geometry shown in Figure (3.17). Taking two initial guesses, x_i and x_{i-1}, one draws a straight line between $f(x_i)$ and $f(x_{i-1})$ passing through the x-axis at x_{i+1}. ABE and DCE are similar triangles. Hence

$$\frac{AB}{AE}=\frac{DC}{DE}$$

$$\frac{f(x_i)}{x_i - x_{i+1}} = \frac{f(x_{i-1})}{x_{i-1} - x_{i+1}}$$

Rearranging, it gives the secant method as

$$x_{i+1} = x_i - \frac{f(x_i)(x_i - x_{i-1})}{f(x_i) - f(x_{i-1})}$$

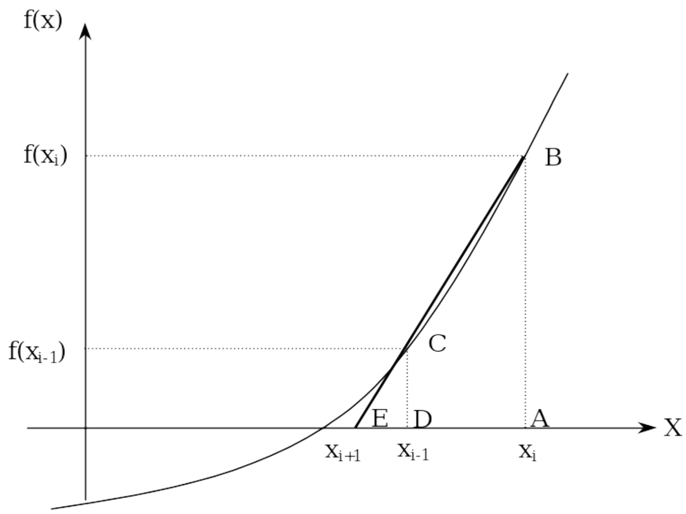


Figure.3.17. Geometrical representation of the Secant method.

VII.1. Difference between the secant and false-position method

In the false position method, the latest estimate of the root replaces whichever of the original values yielded a function value with the same sign as $f(x_r)$. The root is always bracketed by the bonds and the method will always converge.

For the secant method, x_{i+1} replaces x_i and x_i replaces x_{i-1}. As a result, the two values can sometimes lie in the same side of the root and lead to divergence. But when, the secant method converges, it usually does it at a quicker rate.

VIII. Rate of convergence

Figure (3.18) compares the convergence of all the methods.

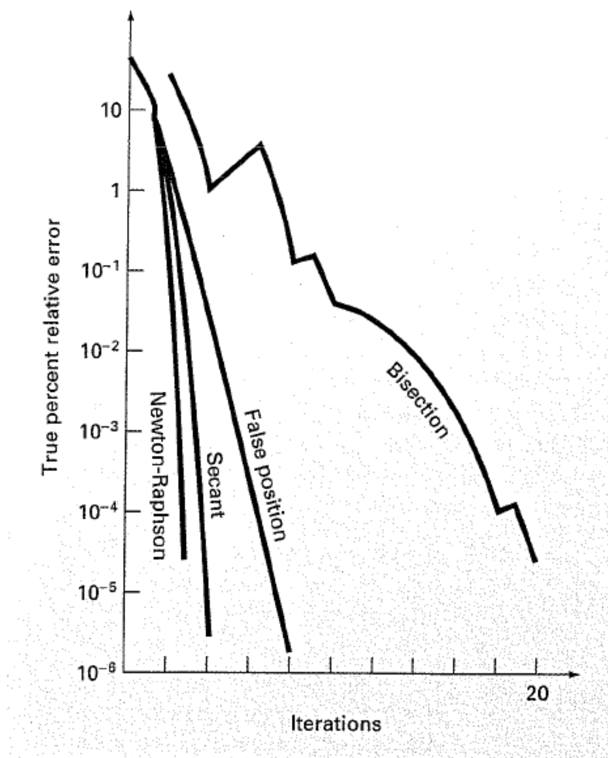


Figure.3.18. Rate of convergence of all the methods.

Additional problems

P I. Find the largest root of:

$$f(x) = x^6 - x - 1 = 0$$

Using the bisection method
(Plot the function first to determine your initial guesses)

Solution: x = 1.1328